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Theoretical study of the electronic properties of semimagnetic superlattices

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We present the first theoretical study of the electronic properties of superlattices formed from semimagnetic semiconductors. We explicitly consider the $Cd_{0.8}Mn_{0.2}Te/Cd_{0.7}Mn_{0.3}Te$ superlattice system. We show magnetic field splittings both including (zero spin temperature) and neglecting (high spin temperature) the exchange interaction. We find that the exchange interaction dominates the magnetic effects. We present calculations of the derivative of the superlattice band gap with magnetic field as a function of the superlattice layer thickness. We show calculations of the change in superlattice band gap with magnetic field for several magnetic fields as a function of temperature.

The growth of high quality $Cd_{1-x}Mn_xTe/Cd_{1-y}Mn_yTe$ superlattices has recently been demonstrated using molecular beam epitaxy techniques.[1–4] Growth has been achieved with both a [111] and [100] growth axis.[5] These materials are particularly interesting because of the presence of the magnetic Mn^{++} ion. The strong exchange interaction between the localized $3d$ electrons of the Mn^{++} ions and itinerant band electrons gives rise to large Zeeman splittings of the energy bands. Magneto-optic studies of these superlattice systems have recently been performed.[6–8] Large magnetic field dependence of the luminescence has been seen. Laser emission has been observed from these superlattices.[9] The energy of the stimulated emission peak has been shifted by application of a magnetic field.

In this letter, we report the first theoretical study of the electronic structure of superlattices formed from semimagnetic semiconductor materials. We consider superlattices made from layers of $Cd_{1-x}Mn_xTe$ with different alloy compositions. The theoretical approach is based on Ref. 10 modified to include the effects of magnetic fields and the exchange interaction in mean field theory using the virtual crystal approximation.[11,12] Parameters describing the average spin state of the Mn^{++} ions as a function of magnetic field and temperature are taken from Ref. 13. The values of the exchange matrix elements are also from Ref. 13. We assume that these matrix elements and spin parameters are the same in the layers forming the superlattice as they are in bulk $Cd_{1-x}Mn_xTe$ alloy. For this material system, the band-gap difference between the two materials is believed to occur primarily in the conduction band.[6,7] Therefore, we take the valence-band offset to be zero. We specifically consider the superlattice system $Cd_{0.8}Mn_{0.2}Te/Cd_{0.7}Mn_{0.3}Te$. The $x = 0.2$ alloy has a smaller band gap and is therefore the quantum well material for electrons. We neglect the small lattice constant difference between the two materials ($\Delta a/a \sim 0.25\%$). Momentum matrix elements and the spin-orbit interaction parameter are taken to be the same in the two constituent materials and to be equal to those of CdTe given in Ref. 14. The band gaps of the constituent materials are from Ref. 15. We consider materials with a [100] growth axis. The magnetic field is taken to be parallel to the growth axis.

For bulk zinc blende semiconductors with a uniform magnetic field in the z direction and a gauge choice so that the vector potential is in the x direction, quantum numbers include the wave vectors k_x, k_z and a Landau level index N. The zeroth order wave functions have the form

$$\psi(\mathbf{r}) = e^{i(k_x X + k_z Z)} \sum_d C_d h_{n_{dN}}(y') U_d(\mathbf{r}),$$

where

$$y' = y - \hbar c k_x / eB. \tag{1}$$

Here C_d is an expansion coefficient, h_n is a harmonic oscillator eigenfunction, U_d is a periodic Kramers basis function, d labels these basis functions, and the index of the harmonic oscillator eigenfunction n depends on both the quantum number N and the basis function d. For a superlattice with B parallel to the growth axis, k_x and N together with a superlattice wave vector Q_z are good quantum numbers. That is, the superlattice wave function is made of a coherent sum of states like that of Eq. (1) in each material. All states in the sum have the same energy, k_x and N; the sum is over k_z which may be complex. Imposing matching conditions at the superlattice interfaces and considering the superlattice translational symmetry in the z direction gives an eigenvalue equation from which one determines the superlattice wave functions and dispersion relations. The exchange interaction, treated in a mean field theory, greatly increases the size

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of the spin splittings produced by the magnetic field, but it does not change the symmetry of the problem.

In Fig. 1, we show the lowest conduction-band and highest valence-band energy levels at $Q_z = 0$ for a superlattice consisting of six molecular layers of each constituent material for three cases: no magnetic field, a magnetic field of 5 T neglecting the exchange interaction (high spin temperature), and a magnetic field of 5 T including the exchange interaction (at zero spin temperature[16]). At $B = 0$, the conduction-band states are twofold degenerate and the valence-band states are fourfold degenerate. (Because the valence-band offset is taken to vanish and lattice mismatch is neglected, there is no splitting of the heavy- and light-hole bands.) For the $B = 5$ T and high spin temperature case,[16] all degeneracies are broken, the conduction-band states move to higher energy and the valence-band states to lower energy. However, the size of the splittings and the motion of the levels are quite small. (The splitting of the two conduction-band states and the highest two valence-band states are so small that they are not resolved in Fig. 1.) For the $B = 5$ T and zero spin temperature case, much larger splittings, due to the exchange interaction, occur and the band gap of the superlattice is decreased by the magnetic field. The state labeling follows that of Ref. 17. (In principle, states corresponding to the "a and b" labeling of Ref. 17 are mixed and the more complete labeling scheme described above should be used. However, the mixing is small and the simpler scheme of Ref. 17 is used in Fig. 1.) All states shown are made up primarily of $n = 0$ harmonic oscillator eigenfunctions. The state labeled a(0) has primarily $|S\uparrow\rangle$ atomic character, b(0) has primarily $|S\downarrow\rangle$ character, b(-1) has primarily $|3/2\ -3/2\rangle$ character, a(-1) has primarily $|3/2\ -1/2\rangle$ character, b(1) has primarily $|3/2\ 1/2\rangle$ character, and a(1) has primarily $|3/2\ 3/2\rangle$ character. The unlabeled lines indicate the energy levels of states made primarily from $n = 1$ harmonic oscillator functions. The positions of states made primarily from higher harmonic oscillator functions are not shown. It is clear from Fig. 1 that the magnetic field splittings in this superlattice are dominated by the exchange interaction.

In Fig. 2, the derivative of the superlattice band gap with magnetic field at small magnetic fields and zero spin temperature[16] is shown as a function of the number of molecular layers of the $x = 0.2$ alloy for three ratios of the superlattice layer thicknesses. Also shown, for comparison, are the corresponding derivatives for the two constituent alloys. First notice that the derivative of the $x = 0.3$ alloy is less than that of the $x = 0.2$ alloy. This occurs, according to the results of Ref. 13, because of stronger antiferromagnetic coupling in the $x = 0.3$ alloy. That is, the net Mn^{++} spin (absolute value of the composition times the average spin $x\langle S_z\rangle$) is larger in the $x = 0.2$ alloy than in the $x = 0.3$ alloy at zero spin temperature and small magnetic fields. The derivatives in the superlattice lie between those of the alloys. For the thin layer superlattices, the alloy results are simply averaged. That is, the 1:1 superlattice result is halfway between the $x = 0.2$ and $x = 0.3$ alloys; the 2:1 superlattice is 1/3 and 1:2 superlattice is 2/3 of the way between the $x = 0.2$ and $x = 0.3$ alloys. For these thin layer superlattices, the electron and hole wave functions are not well confined by energy

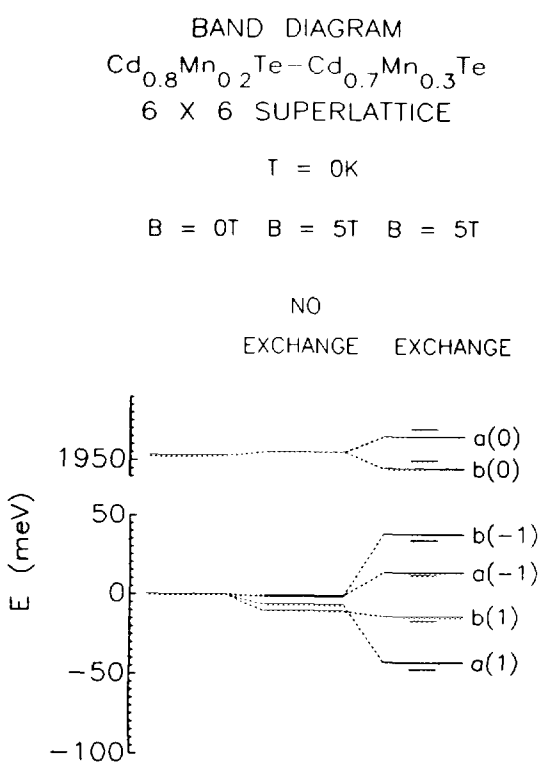

FIG. 1. Energy levels of the lowest conduction-band and highest valence-band states of the superlattice consisting of six molecular layers each of $Cd_{0.8}Mn_{0.2}Te$ and $Cd_{0.7}Mn_{0.3}Te$ for $B = 0$, $B = 5$ T, and no exchange interaction, $B = 5$ T with exchange interaction.

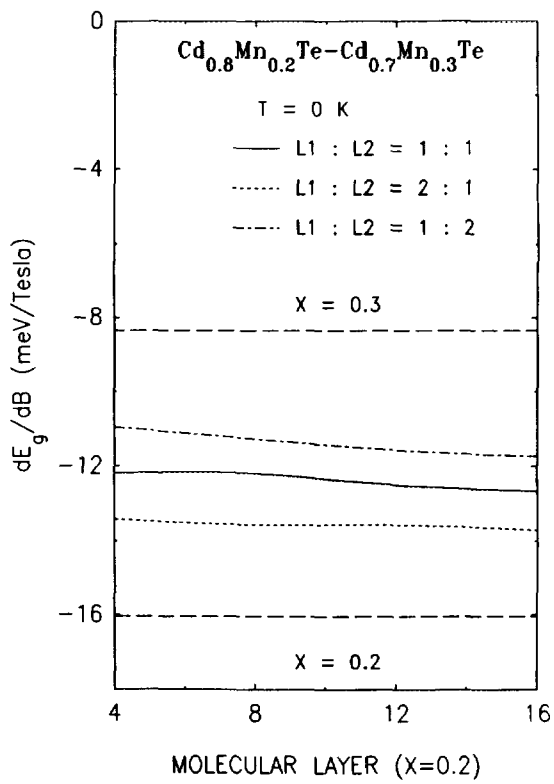

FIG. 2. Derivative of the $Cd_{0.8}Mn_{0.2}Te/Cd_{0.7}Mn_{0.3}Te$ superlattice band gap with magnetic field as a function of the $x = 0.2$ alloy layer thickness for three layer thickness ratios. The corresponding derivatives for the $x = 0.2$ and $x = 0.3$ alloys are shown as straight lines.

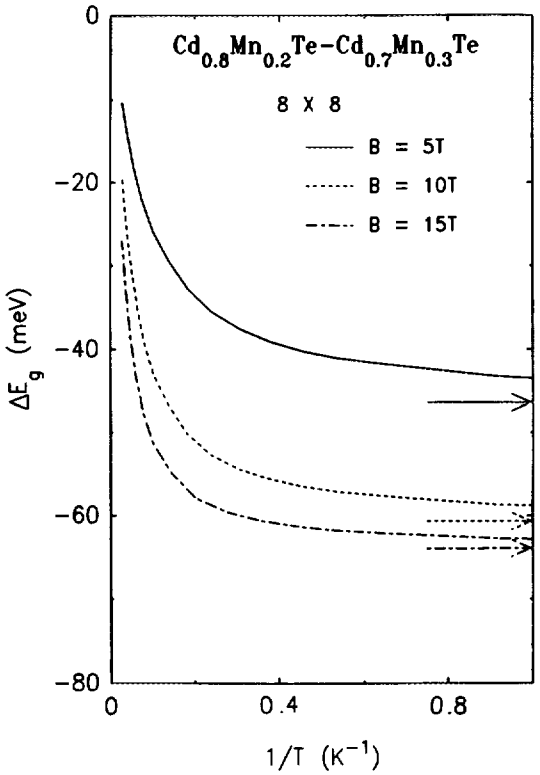

FIG. 3. Change in band gap of the 8×8 $Cd_{0.8}Mn_{0.2}Te/Cd_{0.7}Mn_{0.3}Te$ superlattice as a function of inverse temperature and three magnetic fields. Arrows indicate the zero temperature asymptotes.

barriers. Indeed, the only barrier for holes is due to the exchange interaction itself, like the "spin superlattices" of Ref. 18. As the superlattice layer thicknesses increase, the magnitude of the derivative increases, moving toward the value of the $x = 0.2$ alloy. This occurs because the carrier wave functions are better confined in the $x = 0.2$ alloy in the thicker layer superlattices. The effect is not very large, however, because the barrier for holes is small and the exchange interaction is larger for holes than for electrons.

In Fig. 3, we show the change in band gap with magnetic field at three magnetic fields for a superlattice consisting of eight molecular layers of each alloy as a function of inverse temperature.[16] The arrows indicate the zero temperature asymptotes. The band-gap reduction is due to the exchange interaction of the band electrons with localized $3d$ electrons on Mn^{++}. At low temperatures the Mn^{++} spins align in the direction opposite to the magnetic field leading to a net interaction with the band electrons. At higher temperatures, the Mn^{++} spins are randomized and there is no net exchange interaction with the band electrons (within mean field theory). From the figure, one sees that the strength of the net exchange interactions decreases rapidly with increasing temperature for temperatures above about 5 K.

In summary, we have presented the first theoretical study of the electronic properties of superlattices formed from semimagnetic semiconductors. We have explicitly considered the $Cd_{0.8}Mn_{0.2}Te/Cd_{0.7}Mn_{0.3}Te$ superlattice system. We found that the exchange interaction dominates magnetic effects. The exchange interaction matrix element is larger for holes than for electrons. In this material system, the valence-band offset is small. As a result, holes are not strongly confined in the small band-gap ($x = 0.2$ alloy) material layers and the magnetic properties of the superlattice are similar to that of an alloy.

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